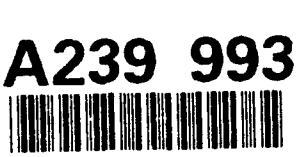

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# Ground-State Properties of a $^3$He Impurity in Liquid $^4$He Monolayers

by

C. I. Um, S. K. Yoo and Thomas F. George

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# Ground-State Properties of a $^3$He Impurity in Liquid $^4$He Monolayers

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## I. Introduction

In the past three decades there has been considerable interest in single-component Bose-fluid[1] and binary boson mixtures[2] at very low temperatures, such as stable bulk spin-polarized hydrogen atom and its isotope.[3] Among the Bose systems, liquid $^4$He and $^3$He-$^4$He mixtures have been analyzed successfully by introducing a Jastrow-type wavefunction. In the investigation of ground states, the Green's function Monte Carlo (GFMC) technique,[4-5] paired-phonon analysis (PPA),[6-7] average correlation approximation (ACA)[8] and hypernetted-chain (HNC) approximation scheme[9-10] provide powerful tools in both two and three dimensions. First, three calculations give the exact ground- and excited-state energies, but less information about the optimized correlation function and other quantities which depend on the long-range behavior, although much experimental data about them have been reported. However, in spite of its weakness in the calculation of the ground-state energy, the HNC approximation can be improved by including the triplet correlation function and some elementary diagrams[11] in the energy and Euler-Lagrange equations.[12-17] Woo and Coldwell[12-13] have considered the wavefunction consisting of the Jastrow function multiplied by a three-particle function and obtained the improved energy and liquid structure function. Recently, Fabrocini and Polls[16] have extended this idea to the ideal boson $^3$He-$^4$He mixture in the zero $^3$He concentration limit.

In the two-dimensional case, Miller and Woo[18] have studied the ground state of a $^4$He monolayer assuming no significant modifications by the existence of a substrate in the mobile limit. Chang[7] has evaluated the ground-state energy and liquid structure function using the optimal Jastrow function determined from a self-consistent PPA, and Hatzikonstantinou[10] has also investigated ground-state properties by using a Jastrow-type wavefunction and solving a Euler-Lagrange equation within the HNC approximation without a three-particle factor.

The main purpose of the present paper is to evaluate the ground-state properties of two-dimensional $^4$He and $^3$He-$^4$He mixtures in the zero $^3$He concentration limit by optimizing a Jastrow-type wavefunction and solving the Euler-Lagrange equations within the HNC approximation, including a triplet correlation function and elementary diagrams up to fifth order.

In Sec. II, we summarize the construction of the Euler-Lagrange equations for zero $^3$He concentration obtained from the energy minimization condition. The Jastrow wavefunction consisting of the product of the two- and three-body correlation factors and the Jackson and Feenberg energy form are adopted. We apply our results to the $^4$He monolayer and the $^3$He-$^4$He mixture in Sec. III to obtain the ground-state energies, radial distribution functions, liquid structure functions and the effective potential, assuming a Lennard-Jones 6-12 potential. The improvements in the ground-state energies and other quantities are also discussed. In Sec. IV, we make conclusions.

## II. Euler-Lagrange Equation in the Zero-Concentration Limit

In this section we consider a homogeneous binary boson mixture, which can be described the the Hamiltonian

$$H = -\frac{\hbar^2}{2m_\alpha}\sum_{i=1}^{N_\alpha}\nabla_i^2 - \frac{\hbar^2}{2m_\beta}\sum_{i=1}^{N_\beta}\nabla_i^2$$

$$+\sum_{i<j}^{N_\alpha} V_{\alpha\alpha}(r_{ij}) + \sum_{i<j}^{N_\beta} V_{\beta\beta}(r_{ij}) + \sum_{\substack{i=1\\j=1}}^{N_\alpha,N_\beta} V_{\alpha\beta}(r_{ij}) \ . \qquad (2.1)$$

Here, the first two terms are kinetic energies of components $\alpha$ and $\beta$, respectively, and $V_{\alpha\beta}(r)$ is the pairwise interaction potential for the three different pairs of particles. We assume that the total number of particles in an area A is $N = N_\alpha + N_\beta$. We choose the Jastrow-type wavefunction in terms of two- and three-particle correlation functions of the form

$$\Psi(\vec{r}_{\alpha,1}, \ldots, \vec{r}_{\alpha,N_\alpha} : \vec{r}_{\beta,1}, \ldots, \vec{r}_{\beta,N_\beta}) = \prod_{i<j} f^{(2)}_{\alpha\alpha}(\vec{r}_{ij}) \prod_{i<j} f^{(2)}_{\beta\beta}(\vec{r}_{ij}) \prod_{\substack{i=1 \\ j=1}}^{N_\alpha N_\beta} f^{(2)}_{\alpha\beta}(\vec{r}_{ij})$$

$$\times \prod_{i<j<k} f^{(3)}_{\alpha\alpha\alpha}(\vec{r}_i,\vec{r}_j,\vec{r}_k) \prod_{i<j<k} f^{(3)}_{\beta\beta\beta}(\vec{r}_i,\vec{r}_j,\vec{r}_k) \prod_{i<j<k} f^{(3)}_{\alpha\alpha\beta}(\vec{r}_i,\vec{r}_j,\vec{r}_k) \prod_{i<j<k} f^{(3)}_{\beta\beta\alpha}(\vec{r}_i,\vec{r}_j,\vec{r}_k)$$

$$= \exp\{\tfrac{1}{2}[ \sum_{i<j} u_{\alpha\alpha}(|\vec{r}_{\alpha,i} - \vec{r}_{\alpha,j}|) + \sum_{i<j} u_{\beta\beta}(|\vec{r}_{\beta,i} - \vec{r}_{\beta,j}|)$$

$$+ \sum_{i<j} u_{\alpha\beta}(|\vec{r}_{\alpha,i} - \vec{r}_{\beta,j}|)\}\exp\{\tfrac{1}{6}[ \sum_{i<j<k} u_{\alpha\alpha\alpha}(\vec{r}_{\alpha,i},\vec{r}_{\alpha,j},\vec{r}_{\alpha,k})$$

$$+ \sum_{i<j<k} u_{\beta\beta\beta}(\vec{r}_{\beta,i},\vec{r}_{\beta,j},\vec{r}_{\beta,k}) + \sum_{i<j<k} u_{\alpha\alpha\beta}(\vec{r}_{\alpha,i},\vec{r}_{\alpha,j},\vec{r}_{\beta,k})$$

$$+ \sum_{i<j<k} u_{\beta\beta\alpha}(\vec{r}_{\beta,i},\vec{r}_{\beta,j},\vec{r}_{\alpha,k})] \quad , \tag{2.2}$$

where $u_{\alpha\beta}(r)$ is the two-body correlation function which satisfies the boundary conditions

$$\lim_{r\to 0} u_{\alpha\beta}(r) \to \infty$$

$$\lim_{r\to\infty} u_{\alpha\beta}(r) = 0 \quad , \tag{2.3}$$

and $u_{\alpha\beta\gamma}(r)$ is the three-body correlation factor. The two-body distribution function can be defined as

$$g_{\alpha\beta}(r) = \frac{N_\alpha(N_\beta - \delta_{\alpha\beta})}{\rho_\alpha\rho_\beta} \frac{\int d\vec{r}(i_\alpha, i_\beta)\ \Psi^*\Psi}{\int d\vec{r}_1 \ldots d\vec{r}\ \Psi^*\Psi} \quad , \tag{2.4}$$

where $d\vec{r}(i_\alpha, i_\beta)$ denotes $d\vec{r}_1 \ldots d\vec{r}_N$ with the exclusion of $d\vec{r}_{i_\alpha}$ and $d\vec{r}_{i_\beta}$, and $\rho_\alpha = N_\alpha/A$ is the partial density of component $\alpha$. The radial distribution function $g^{(2)}_{\alpha\beta}(r)$ must also satisfy the conditions

$$\lim_{r\to\infty} [g_{\alpha\beta}(r) - 1] = 0$$

$$\rho \int d^{2\vec{r}} [g_{\alpha\beta}(r) - 1] + \delta_{\alpha\beta} = 0 \quad . \tag{2.5}$$

Defining $x_\alpha = \rho_\alpha/\rho$ as the concentration of component $\alpha$, where $\rho = (N_\alpha + N_\beta)/A$ is the total density, we can express the energy per particle of the system as

$$E = E^{(2)} + E^{(3)} \quad , \tag{2.6}$$

with

$$E^{(2)} = x_\alpha^2 E_{\alpha\alpha} + 2x_\alpha x_\beta E_{\alpha\beta} + x_\beta^2 E_{\beta\beta} \quad . \tag{2.7}$$

and

$$E^{(3)} = x_\alpha^3 E_{\alpha\alpha\alpha} + 3[x_\alpha^2 x_\beta E_{\alpha\alpha\beta} + x_\alpha x_\beta^2 E_{\beta\beta\alpha}] + x_\beta^3 E_{\beta\beta\beta} \quad . \tag{2.8}$$

The two- and three-body energies are

$$E^{(2)}_{\alpha\beta} = \frac{1}{2}\rho \int d^2\vec{r}\; g^{(2)}_{\alpha\beta}(r)\bar{v}_{\alpha\beta}(r) \quad , \tag{2 9}$$

with the effective interaction

$$\bar{v}_{\alpha\beta}(r) = V_{\alpha\beta}(r) - \frac{\hbar^2}{4m_{\alpha\beta}}\nabla^2 u_{\alpha\beta}(r)$$

$$m_{\alpha\beta}^{-1} = \frac{1}{2}(m_\alpha^{-1} + m_\beta^{-1}) \quad , \tag{2.10}$$

and

$$E^{(3)}_{\alpha\beta\gamma} = \frac{1}{6}\rho \int d\vec{r}\; g^{(3)}_{\alpha\beta\gamma}(\vec{r}_\alpha,\vec{r}_\beta,\vec{r}_\gamma)V_{\alpha\beta\gamma}(r) \quad , \tag{2.11}$$

with

$$V_{\alpha\beta\gamma}(r) = \frac{\hbar^2}{+}[\frac{\nabla_\alpha^2}{m_\alpha} + \frac{\nabla_\beta^2}{m_\beta} + \frac{\nabla_\gamma^2}{m_\gamma}]U^{(3)}_{\alpha\beta\gamma}(\vec{r}_\alpha,\vec{r}_\beta,\vec{r}_\gamma) \quad , \tag{2.12}$$

where $g^{(3)}_{\alpha\beta\gamma}(\vec{r}_\alpha,\vec{r}_\beta,\vec{r}_\gamma)$ is the three-body distribution function. This is written as

$$g_{\alpha\beta\gamma}(\vec{r}_\alpha,\vec{r}_\beta,\vec{r}_\gamma) = g^{(2)}_{\alpha\beta}(r_{\alpha\beta})g^{(2)}_{\gamma\alpha}(r_{\gamma\alpha})g^{(2)}_{\gamma\beta}(r_{\gamma\beta})$$

$$\times [f^{(3)}(\vec{r}_\alpha,\vec{r}_\beta,\vec{r}_\gamma)]^2\; e^{A(\vec{r}_\alpha,\vec{r}_\beta,\vec{r}_\gamma)} \quad , \tag{2.13}$$

where $A(\vec{r}_\alpha,\vec{r}_\beta,\vec{r}_\gamma)$ is the sum of the contributions of all the Abe terms.

In order to establish a relation between $g^{(2)}_{\alpha\beta}(r)$ and $f^{(2)}_{\alpha\beta}(r)$, we introduce the HNC approximation, which consists of the equation[1]

$$g^{(2)}_{\alpha\beta}(r) = [f^{(2)}_{\alpha\beta}(r)]^2 \exp[C_{\alpha\beta}(r) + T_{\alpha\beta}(r) + E_{\alpha\beta}(r)] \quad , \tag{2.14}$$

where

$$C_{\alpha\beta}(r) = \sum_i \rho_i \int d\vec{r}_i \; [g^{(2)}_{\alpha\beta}(r) - 1 - C_{\alpha\beta}(r)][g^{(2)}_{\alpha\beta}(r) - 1] \quad , \tag{2.15}$$

$T_{\alpha\beta}(r)$ is the integral of the triplet function

$$T_{\alpha\beta}(r) = \sum_i \rho_i \int d\vec{r}_i \; [g^{(2)}_{\alpha\beta}(r_{ij}) g^{(2)}_{\alpha\beta}(r_{ik})([f^{(3)}_{\alpha\beta\gamma}(\vec{r}_i,\vec{r}_j,\vec{r}_k)]^2 - 1) \quad , \tag{2.16}$$

and $E_{\alpha\beta}(r)$ is the sum of all the elementary diagrams. Rewriting Eq. (2.9) and taking $C_{\alpha\beta}(r)$ in momentum space, we get

$$E^{(2)}_{\alpha\beta} = \frac{1}{2}\rho \int d^2\vec{r} \; g^{(2)}_{\alpha\beta}(r) V_{\alpha\beta}(r) - \frac{\hbar^2\rho}{8m_{\alpha\beta}} \int d^2\vec{r} \; g^{(2)}_{\alpha\beta}(r)\nabla^2 \ln g^{(2)}_{\alpha\beta}(r)$$

$$- \frac{\hbar^2\rho}{8m_{\alpha\beta}} \frac{\delta_{\alpha\beta}}{(2\pi)^2\rho_\alpha\rho_\beta} \int d^2\vec{k} \; k^2 \{S_{\alpha\beta}(k)[S_{\alpha\beta}(k) - 3] - 2$$

$$+ \frac{S_{\gamma\beta}(k)[1 - S_{\alpha\beta}(k)]}{D(k)}\} - \frac{\hbar^2\rho}{8m_{\alpha\beta}} \int d^2\vec{r} \; g^{(2)}_{\alpha\beta}(r)\nabla^2[T_{\alpha\beta}(r) + E_{\alpha\beta}(r)] \quad , \tag{2.17}$$

where $S_{\alpha\beta}(k)$ is the liquid structure function of the form

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} + 2\pi\rho \int dr\, r\, [g^{(2)}_{\alpha\beta}(r) - 1]\, J_0(kr) \quad , \tag{2.18}$$

$D(k) = S_{11}S_{22} - S_{12}^2$ and $\alpha \neq \gamma$. Here $J_0(kr)$ is the zeroth-order Bessel function. To minimize the energy, we must calculate the variational equations $\delta E/\delta f^{(2)}(r) = 0$ and $\delta E/\delta f^{(3)}(r) = 0$ and solve the resultant Euler-Lagrange equations. In the presence of triplet correlations this is very complicated. To solve this problem we take the limit of zero concentration of component $\alpha$ and assume that $f^{(3)}(r)$ is fixed for all the triplets. Minimizing the energy, we finally get the Euler-Lagrange equations

$$[-\frac{\hbar^2}{m_{\alpha 2}}\nabla^2 + V_{\alpha 2}(r) + W^0_{\alpha 2}(r) + W^T_{\alpha 2}(r) + W^E_{\alpha 2}(r)][g^{(2)}_{\alpha 2}(r)]^{\frac{1}{2}} = 0 \quad , \tag{2.19}$$

where $\alpha = 1,2$. Here $W^0_{\alpha 2}(r)$, $W^T_{\alpha 2}(r)$ and $W^E_{\alpha 2}(r)$ are the induced potentials due to two-body correlations, triplet correlations and elementary diagrams, respectively. $W^0_{\alpha 2}(r)$ is expressed in momentum space as

$$W^0_{12}(k) = -\frac{\hbar^2 k^2}{4m_2\rho_2}\frac{S_{12}(S_{22} - 1)}{S^2_{22}}(2m_{12}^{-1}m_2 S_{22} + 1)$$

$$W^0_{22}(k) = -\frac{\hbar^2 k^2}{4m_2\rho_2}\frac{(S_{22} - 1)^2(2S_{22} + 1)}{S^2_{22}} \quad , \tag{2.20}$$

and

$$W^T_{\alpha 2}(r) = \frac{\hbar^2}{8m_{\alpha 2}}\nabla^2 T_{\alpha 2}(r) \quad . \tag{2.21}$$

$$W^E_{\alpha 2}(r) = \frac{\hbar^2}{8m_{\alpha 2}}\nabla^2 E_{\alpha 2}(r) \quad . \tag{2.22}$$

Here we assume $E_{12}(r) = E_{21}(r)$. We may rewrite Eq. (2.6) for slight changes in $x_1$ as

$$E^{(2)} = E_{22}^{(2)} + 2x_1[E_{12}^{(2)} - E_{22}^{(2)}] + x_1^2[E_{11}^{(2)} - 2E_{12}^{(2)} + E_{22}^{(2)}] \quad . \tag{2.23}$$

Assuming that there is an impurity in the mixture, then $x_1$ would be 1/N, and approximately to order 1/N we can minimize $E^{(2)}$ through minimization of $E_{22}(r)$, that is $g_{\alpha\beta}^{(2)}(r)$ can be estimated consecutively.

From the Euler-Lagrange equations we can construct the n-th step iteration scheme and find $g_{\alpha 2,n+1}^{(2)}(r) = g_{\alpha 2,n}^{(2)}(r) + \delta g_{\alpha 2,n}^{(2)}(r)$ for a given $g_{\alpha 2,n}^{(2)}(r)$. Then by means of the convolution theorem, the Euler-Lagrange equations can be converted to

$$[\nabla^2 - \frac{m_{\alpha 2}}{\hbar^2}(V_{\alpha 2} + W_{\alpha 2,n}^0 + W_{\alpha 2,n}^T + W_{\alpha 2,n}^E)]\delta g_{\alpha 2,n}^{(2)\frac{1}{2}}(r)$$

$$+ [\nabla^2 - \frac{m_{\alpha 2}}{\hbar^2}(V_{\alpha 2} - W_{\alpha 2,n}^0 - W_{\alpha 2,n}^T - W_{\alpha 2,n}^E)]g_{\alpha 2,n}^{(2)\frac{1}{2}}(r)$$

$$+ g_{\alpha 2,n}^{(2)\frac{1}{2}}(r) \int d^2\vec{r}\, W_{\alpha 2,n}^{0\prime}(r - r')g_{\alpha 2,n}^{(2)\frac{1}{2}}(r')\delta g_{\alpha 2,n}^{(2)\frac{1}{2}}(r') = 0 \quad . \tag{2.24}$$

where $W_{\alpha 2}'$ is given by

$$W_{12}^{0\prime} = \frac{k^2[2m_{12}^{-1}m_2 S_{22}^2 + (1 - 2m_{12}^{-1}m_2)S_{22} - 1]}{S_{22}^2}$$

$$W_{22}^{0\prime} = \frac{k^2(S_{22}^3 - 1)}{2S_{22}^3} \quad . \tag{2.25}$$

This variational calculation consists of two parts: (a) we consider a system of a background component and a trial wavefunction of the form of Eq. (2.2) and determine $g_{22}^{(2)}(r)$ variationally, and (b) we replace the background system with an impurity and introduce the trial wavefunction

$$\Psi(\vec{r}_1,\ldots,\vec{r}_{n-1},\vec{r}_n) = \exp\{\tfrac{1}{2}[\sum_{i<j}^{n-1} u_{22}(r_{ij}) + \sum_{k=1}^{n-1} u_{12}(r_{kn})]\}$$

$$\times \exp\{\tfrac{1}{6}[\sum_{i<j<k}^{n-1} u_{222}(\vec{r}_i,\vec{r}_j,\vec{r}_k) + \sum_{i<j=k}^{n-1} u_{221}(\vec{r}_i,\vec{r}_j,\vec{r}_n)]\} \quad . \tag{2.26}$$

Through step (b), $g_{12}^{(2)}(r)$ can be determined variationally.

Equation (2.24) represents a set of integro-differential equations. Under the assumption that $\delta g_{\alpha 2}^{(2)}(r)$ vanishes outside some radius R, Eq. (2.24) can be replaced by a finite sum over a set of equally-spaced points in coordinate space, and the Laplacian term for $\delta g_{\alpha 2}^{(2)}(r)$ can also be expressed by finite differences. Then we get a set of inhomogeneous linear equations, which can be written in matrix form and diagonalized by the standard Gauss elimination technique. By making a good choice for the initial $g_{\alpha 2}^{(2)}(r)$, the rate of convergence will be rapid, so that the optimized distribution function can be readily obtained.

## III. Numerical Results and Discussion

In this section we apply the results obtained in previous sections to two-dimensional $^3$He and (Bose)$^3$He-$^4$He mixtures in the zero $^3$He concentration limit. To be realistic in the two-dimensional mixture, it is necessary to consider the $^3$He coverage of a few atomic layers on the $^4$He background.[19] At T = 0 K a $^3$He particle behaves nearly like $^4$He particle, and thus we assume that the potential $V_{\alpha\beta}(r)$

appearing in the Hamiltonian [Eq. (2.1)] are all of the form of a Lennard-Jones potential given as

$$V_{\alpha\beta}(r) = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}] \quad , \tag{3.1}$$

with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å. As an initial trial guess for $g_{22}^{(2)}(r)$, we adopt the results for $g_{22}^{(2)}(r)$ and $S_{22}(k)$ obtained from the Jastrow wavefunction, which are only known for $r \leq 5$ Å and $k \leq 5$ Å$^{-1}$, such that the short-range behavior of $g(r)$ at a density of 0.03 Å$^{-2}$ coincides with the results obtained from the PPA.[7] The initial form of $g_{22}^{(2)}(r)$ is evaluated using an iterative scheme,[10] since the long-range behavior of $g(r)$ depends on the value of $S(k)$ for small $k$, and the exact value of $S(k)$ for $k \geq 5$Å$^{-1}$ depends on the value of $g(r)$ for small $r$. The initial value of $g_{12}^{(2)}(r)$ is determined by optimizing $g_{22}^{(2)}(r)$.

For the triplet correlation functions we assume that $f^{(3)}(r)$ has the same form for all the triplets and choose the parametrized form given as

$$f^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \exp[\sum_{\text{cyclic}} \lambda\xi(r_{ij})\zeta(r_{ik})r^2\hat{r}_{ij}\cdot\hat{r}_{ik}] \quad . \tag{3.2}$$

with

$$\zeta(r) = F(r)\exp(-[(r-r_t)/w]^2) \tag{3.3}$$

$$F(r \leq b) = [(r - r_b)/r_b]^3 \quad , \qquad F(r > r_b) = 0 \quad .$$

Here $\hat{r}_{ij}$ and $\hat{r}_{ik}$ are unit vectors in the direction of radial vectors $\vec{r}_{ij}$ and $\vec{r}_{ik}$, respectively. We choose the parameters $r_b$, $r_t$, $\lambda$ and $\omega$ as those which are adopted in

the three-dimensional case, and note that the energies and radial distribution functions are not significantly affected by the choice of the above parameters. Taking the terms of elementary diagrams up to fifth order with the triplet correlation factor and approximating $E_{12}(r)$ by $E_{22}(r)$, the calculation of the integro-differential equation [Eq. (2.24)] is carried out by using the Gauss elimination technique until r = 20 Å.

The ground-state energies per particle for pure liquid $^4$He and $^3$He-$^4$He mixtures are listed in Table 1. By considering the triplet correlation factor and elementary diagrams, the energies are lowered by about 21-96% compared with those considering the two-body factor only, and the equilibrium density increases for the pure case but decreases for the mixture case. The changes by the triplet correlation and elementary diagrams are shown in Figure 1. For the pure case (solid line), the ground-state energy is -0.646 K at the equilibrium density of $\rho$ = 0.0350 Å$^{-2}$ and similar to the results of the BBGKY,[18] the molecular dynamics[20] and the Monte Carlo studies.[4] For the mixture case (dashed line), the equilibrium density is 0.0336 Å$^{-2}$ with a ground-state energy -0.542 K. The rate of drifts in energies are similar to that in the three-dimensional system. Moreover, we can view the chemical potential of $^3$He at T = 0 K as independent of the density of the $^4$He background due to complete phase separation.[8]

We note that one of us (CIU) has evaluated the ground-state energies of one- and two-dimensional Bose liquids[21] and charged boson systems using ring diagrams[22] and the self-consistent field approximation.[23] In these results the ground-state energies of one- and two-dimensional Bose fluids consist of repulsive and attractive parts with the adoption of a soft potential with a Lennard-Jones tail. For our current two-dimensional boson system, the ground-state energy is proportional to $R_a^{-2/3}$ with an additive positive constant, where $R_a$ is the ratio of the mean

separation between particles to the Bohr radius within the self-consistent approximation. This result is different from that of the ring diagram approximation, which does not include an additive positive constant.

Figure 2 illustrates the optimal radial distributions of $g_{22}^{(2)}(r)$ (dashed line) and $g_{12}^{(2)}(r)$ (solid line) at the respective equilibrium density, while their numerical values at various density are listed in Table 2. As the density increases, the maximum values of $g_{22}^{(2)}(r)$ and $g_{12}^{(2)}(r)$ increase. At the equilibrium density the maximum position of $g_{12}^{(2)}(r)$ shifts to the right (direction of increasing radial distance) in comparison with the fixed $g_{22}^{(2)}(r)$. This behavior is due to the fact that the volume swept by $^3$He is larger than that by $^4$He. The maximum value of $g_{12}^{(2)}(r)$ is smaller than that of $g_{22}^{(2)}(r)$ and broadened around the maximum point because of less localization of the $^3$He impurity with a larger zero-point energy. In this sense the behavior of $g_{12}^{(2)}(r)$ agrees with the three-dimensional case.[23] With the consideration of the triplet correlation function, the maxima of $g_{12}^{(2)}(r)$ and $g_{22}^{(2)}(r)$ increase but are hardly affected by elementary diagrams. However, the ground-state energies are lowered not only by triplet factors but by elementary diagrams. We note that the optimized radial distribution functions[21,22,25] of one-, two- and three-dimensional hard-sphere Bose systems decrease as $r^{-2}$, $r^{-3}$ and $r^{-4}$, respectively, at short distances, while at long distances they oscillate and tend to go to unity as $r \to \infty$, which is due to the contribution from the core part of the soft potential. These three proportionalities represent the main long-distance behaviors of phonons in each dimensional Bose liquid.

Figure 3 shows the optimized liquid structure functions at various densities. The initial slope decreases, which implies a decrease of sound velocity, but the maximum increases and shifts to the right with increasing density. A comparison between $S_{12}(k)$ (solid line) and $S_{22}(k) - 1$ (dashed line) at equilibrium density is shown in Figure 4. The addition of the impurity $^3$He leads to a decrease of the

maximum and shift of the maximum position to the right in k-space. This behavior obtained is as expected in a scattering problem and agrees with that of the three-dimensional case[25] except in the region of $k \to 0$.

In Figure 5 we plot the bare Lennard-Jones potential $V_{LJ}$, the induced potential $W_{12}(r)$ ($V_{ind}$) and the effective potential $V_{eff}$. According to Table 3, we observe for the effective potential that as the density increases, its hard core radius ($V_{eff} = 0$) decreases and potential becomes deeper, while the repulsive barrier height grows at about the same position.

## IV. Conclusions

We have investigated the ground-state properties and behaviors of the $^3$He-$^4$He system. The introduction of the triplet correlation and elementary diagrams up to fifth order in the HNC approximation leads to successful improvement in the ground-state energy and optimized two-body distribution functions. Furthermore, the triplet correlation factor contributes to the change of both energy and the distribution function, while elementary diagrams do not change the distribution function. By addition of an impurity $^3$He into a $^4$He background, the energy increases, the distribution function moves to the right, and its maximum decreases and is broadened around the maximum position, due to larger zero-point energy and less localization of the $^3$He particle.

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Table 1. Ground-state energies $E_0$ due to the two-body factor only (2), two- and three-body factors (2+3) and two- and three-body factors plus elementary diagrams (tot) for the pure and mixture cases at various densities.

| $\rho$ ($Å^{-2}$) | $E_{0,mix}(2)$ (K) | $E_{0,mix}(2+3)$ (K) | $E_{0,mix}(tot)$ (K) | $E_{0,pure}(2)$ (K) | $E_{0,pure}(2+3)$ (K) | $E_{0,pure}(tot)$ (K) |
|---|---|---|---|---|---|---|
| 0.0250 | -0.28 | -0.38 | -0.45 | -0.39 | -0.45 | -0.50 |
| 0.0275 | -0.30 | -0.40 | -0.48 | -0.44 | -0.48 | -0.55 |
| 0.0300 | -0.32 | -0.43 | -0.50 | -0.48 | -0.53 | -0.58 |
| 0.0325 | -0.35 | -0.45 | -0.53 | -0.46 | -0.56 | -0.62 |
| 0.0350 | -0.38 | -0.47 | -0.54 | -0.46 | -0.59 | -0.65 |
| 0.0375 | -0.35 | -0.45 | -0.52 | -0.43 | -0.58 | -0.63 |
| 0.0400 | -0.33 | -0.44 | -0.51 | -0.40 | -0.57 | -0.61 |

Table 2. Radial distribution functions at various densities.

| | $\rho$ = 0.025 Å$^{-2}$ | | $\rho$ = 0.030 Å$^{-2}$ | | $\rho$ = 0.035 Å$^{-2}$ | |
|---|---|---|---|---|---|---|
| r(Å) | $g_{22}(r)$ | $g_{12}(r)$ | $g_{22}(r)$ | $g_{12}(r)$ | $g_{22}(r)$ | $g_{12}(r)$ |
| 2.0 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 2.2 | 0.010 | 0.010 | 0.010 | 0.011 | 0.010 | 0.011 |
| 2.4 | 0.067 | 0.065 | 0.070 | 0.066 | 0.071 | 0.069 |
| 2.6 | 0.208 | 0.207 | 0.211 | 0.209 | 0.215 | 0.209 |
| 2.8 | 0.409 | 0.404 | 0.418 | 0.408 | 0.425 | 0.413 |
| 3.0 | 0.628 | 0.608 | 0.640 | 0.621 | 0.656 | 0.630 |
| 3.2 | 0.835 | 0.801 | 0.839 | 0.815 | 0.841 | 0.828 |
| 3.4 | 0.988 | 0.960 | 0.992 | 0.963 | 0.997 | 0.970 |
| 3.6 | 1.086 | 1.055 | 1.095 | 1.066 | 1.101 | 1.075 |
| 3.8 | 1.140 | 1.109 | 1.159 | 1.117 | 1.160 | 1.126 |
| 4.0 | 1.188 | 1.140 | 1.189 | 1.155 | 1.198 | 1.160 |
| 4.2 | 1.181 | 1.145 | 1.182 | 1.158 | 1.190 | 1.162 |
| 4.4 | 1.169 | 1.131 | 1.168 | 1.135 | 1.173 | 1.140 |
| 4.6 | 1.121 | 1.095 | 1.121 | 1.099 | 1.123 | 1.103 |
| 4.8 | 1.084 | 1.077 | 1.084 | 1.078 | 1.085 | 1.075 |
| 5.0 | 1.050 | 1.048 | 1.043 | 1.043 | 1.043 | 1.040 |
| 5.2 | 1.015 | 1.019 | 1.015 | 1.018 | 1.010 | 1.011 |
| 5.4 | 0.990 | 0.996 | 0.987 | 0.992 | 0.986 | 0.990 |
| 5.6 | 0.972 | 0.978 | 0.969 | 0.974 | 0.967 | 0.972 |
| 5.8 | 0.957 | 0.963 | 0.956 | 0.961 | 0.955 | 0.959 |
| 6.0 | 0.951 | 0.956 | 0.948 | 0.953 | 0.947 | 0.952 |

Table 3. Induced potentials $V_{ind}$ and effective potentials $V_{eff}$ at various densities.

| | $\rho$ = 0.025 Å$^{-2}$ | | $\rho$ = 0.030 Å$^{-2}$ | | $\rho$ = 0.35 Å$^{-2}$ | |
|---|---|---|---|---|---|---|
| r(Å) | $V_{ind}$(K) | $V_{eff}$(K) | $V_{ind}$ | $V_{eff}$ | $V_{ind}$ | $V_{eff}$ |
| 2.4 | -1.056 | 26.332 | -1.625 | 25.763 | -2.401 | 24.987 |
| 2.6 | -0.756 | -4.347 | -1.162 | -4.754 | -1.752 | -5.344 |
| 2.8 | -0.480 | -10.447 | -0.942 | -10.709 | -1.159 | -11.126 |
| 3.0 | -0.226 | -9.882 | -0.367 | -10.023 | -0.623 | -10.279 |
| 3.2 | 0.009 | -7.850 | -0.027 | -7.887 | -0.141 | -8.000 |
| 3.4 | 0.231 | -5.816 | 0.290 | -5.758 | 0.302 | -5.744 |
| 3.6 | 0.437 | -4.129 | 0.579 | -3.987 | 0.702 | -3.863 |
| 3.8 | 0.607 | -2.828 | 0.812 | -2.624 | 1.024 | -2.412 |
| 4.0 | 0.757 | -1.828 | 1.026 | -1.568 | 1.315 | -1.279 |
| 4.2 | 0.950 | -1.021 | 1.279 | -0.692 | 1.643 | -0.329 |
| 4.4 | 1.216 | -0.294 | 1.637 | 0.126 | 2.086 | 0.575 |
| 4.6 | 1.546 | 0.378 | 2.052 | 0.884 | 2.588 | 1.421 |
| 4.8 | 1.828 | 0.917 | 2.364 | 1.453 | 2.964 | 2.053 |
| 5.0 | 1.885 | 1.168 | 2.359 | 1.642 | 2.960 | 2.244 |
| 5.2 | 1.625 | 1.057 | 1.968 | 1.490 | 2.501 | 1.932 |
| 5.4 | 1.123 | 0.669 | 1.328 | 0.874 | 1.745 | 1.291 |
| 5.6 | 0.576 | 0.210 | 0.694 | 0.328 | 0.995 | 0.629 |
| 5.8 | 0.154 | -0.143 | 0.249 | -0.048 | 0.466 | 0.168 |
| 6.0 | -0.088 | -0.331 | -0.022 | -0.221 | 0.191 | -0.052 |

Figure Captions

1. Ground-state energies of the pure $^4$He system (solid line) and (Bose) $^3$He-$^4$He mixture in the impurity $^3$He limit (dashed line) as a function of density. E(2), E(2+3) and E(tot) represent the energy containing the two-body correlation factor only, energy by two- and three-body factors, and total energy by the above factors plus elementary diagrams, respectively.

2. Optimized radial distribution functions $g_{12}^{(2)}(r)$ (solid line) and $g_{22}^{(2)}(r)$ (dashed line) at equilibrium density.

3. Optimized liquid structure function $S_{12}(k)$ at various densities.

4. Optimized liquid structure function $S_{12}(k)$ (solid line) and $S_{22}(k)-1$ (dashed line) at the equilibrium density.

5. Bare Lennard-Jones potential ($V_{LJ}$), induced potential ($V_{ind}$) and effective potential ($V_{eff}$) at the equilibrium density.

Fig. 1

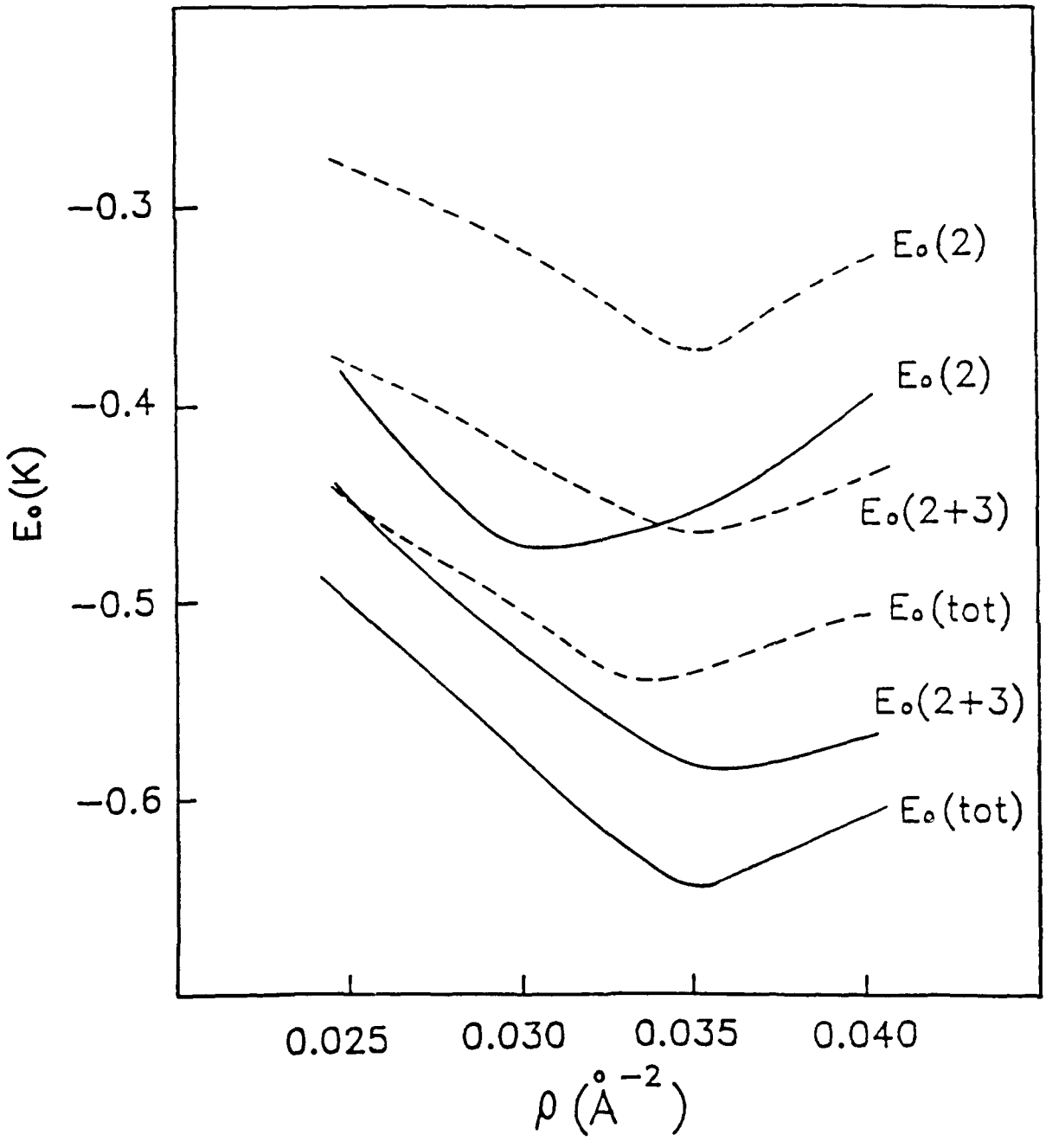
−0.3
−0.4
−0.5
−0.6
E₀(K)
E₀(2)
E₀(2)
E₀(2+3)
E₀(tot)
E₀(2+3)
E₀(tot)
0.025
0.030
0.035
0.040
ρ (Å⁻²)

Fig. 2

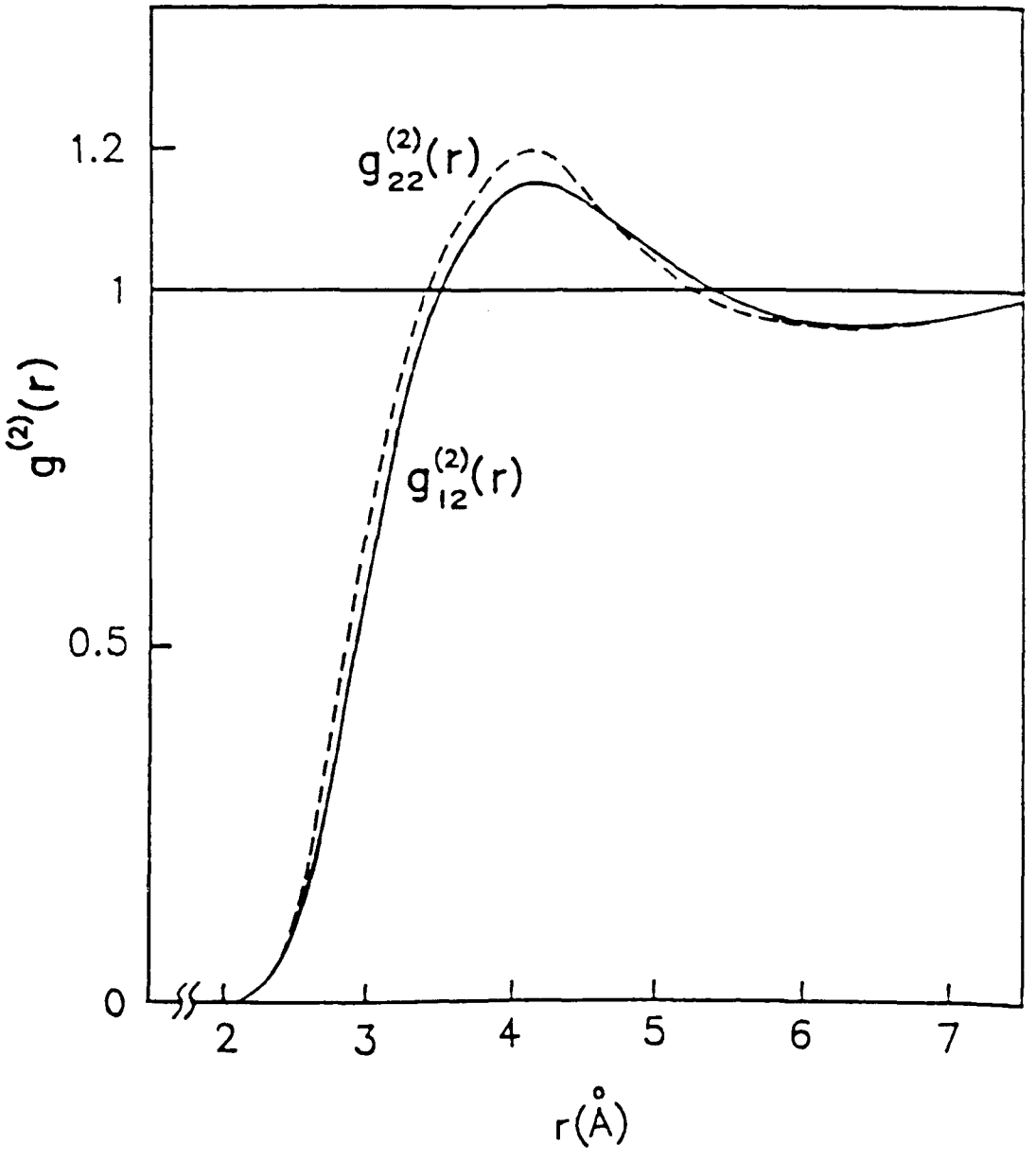

Fig. 3

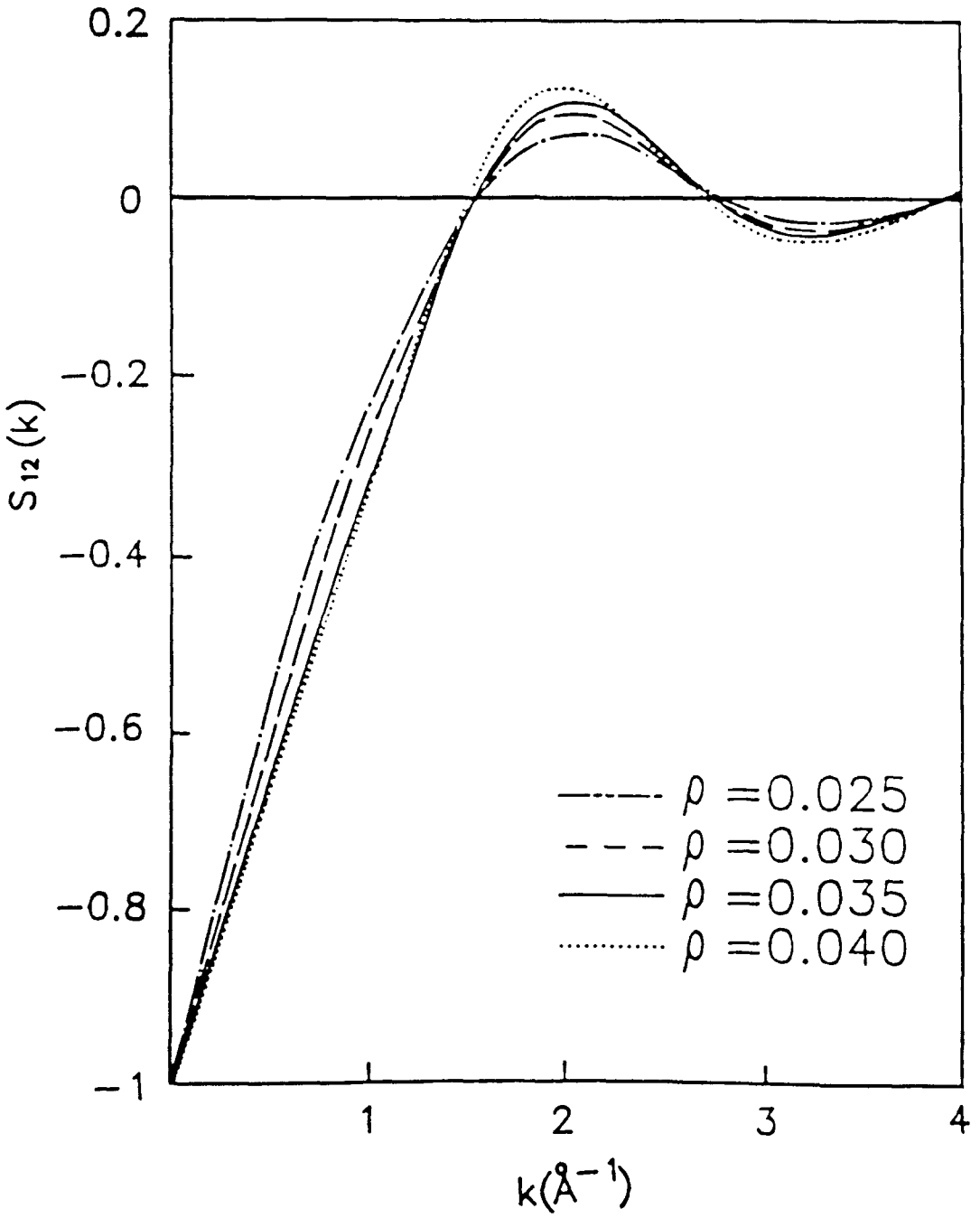

Fig. 4

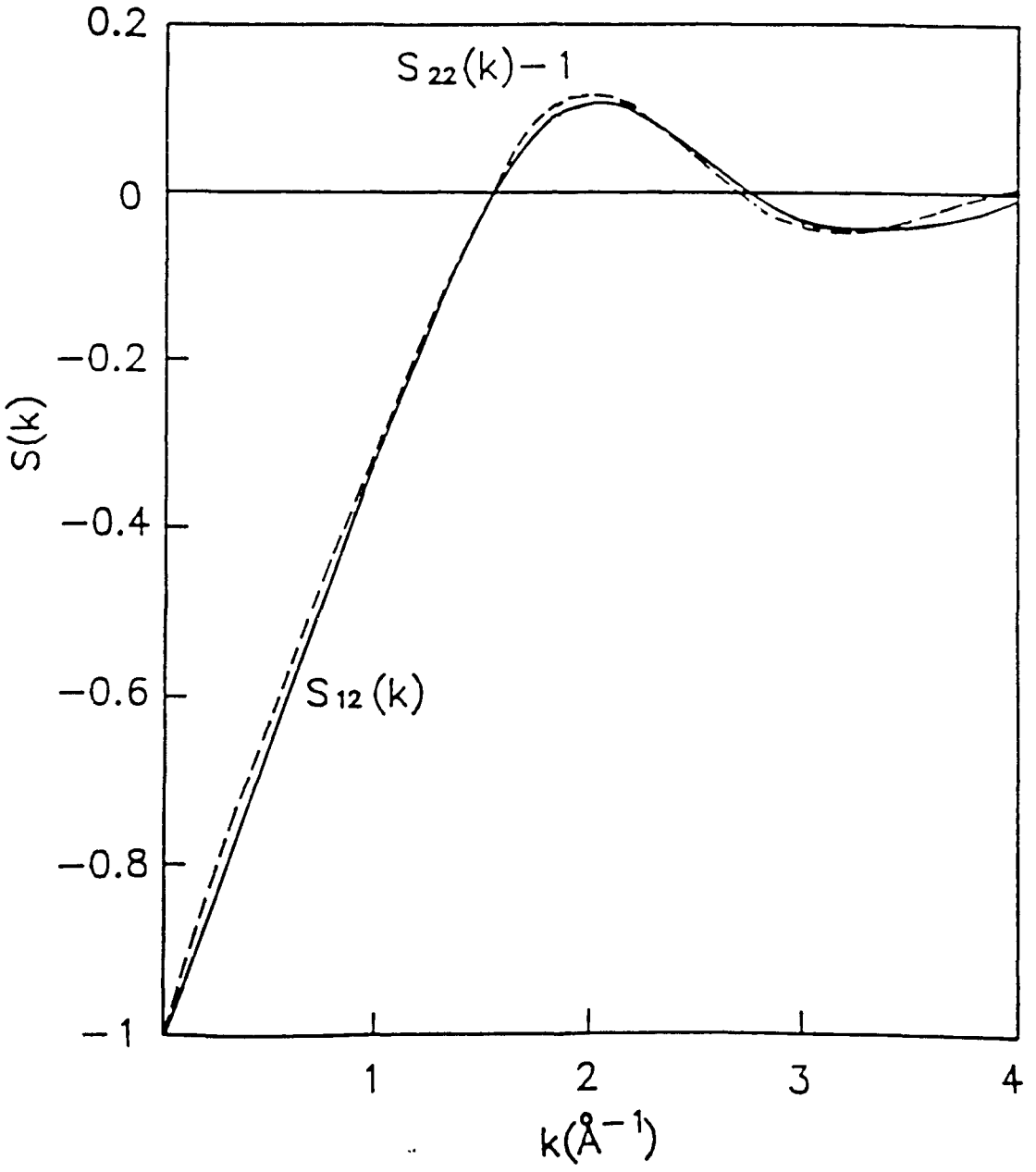

Fig. 5